BRICC Program Package
v 2.0

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(Dated: December 16, 2005)

Abstract

The BRICC program package consists of BLDBRICC and BRICC. The program BLDBRICC builds a direct access file from the tabulated electron and electron–positron pair conversion coefficients, and from the E0 electronic factors. BRICC can be used in different ways: as an interactive tool to interpolate conversion coefficients and E0 electronic factors and as an ENSDF evaluation tool. The program will prepare new ENSDF records (GAMMA and GAMMA continuation) and it also can be used to merge the new cards into existing ENSDF data sets.

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I. THE ENSDF FILE

The Evaluated Nuclear Structure Data File (ENSDF), is a computer-based file system designed to store nuclear structure information. It is maintained by the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory for the international Nuclear Structure and Decay Data Network.

The ENSDF file usually contains a number of data sets, each data set refers to a particular reaction or decay mode of a nucleus. Adopted level and gamma-ray properties for each nuclide are kept in a separate data set. The data sets are composed of 80–character records. The most up–to–date description of the ENSDF files is given by J.K. Tuli [2001TuAA]. Throughout this manual we will frequently make reference to this document. Spectroscopic information is kept in predefined fields of the 80–character records. These fields are marked with bold typeface. For example the numerical value of the total conversion coefficient, stored in the **CC** field of the **GAMMA** record, is α_{tot}.

This document describes the use of the utility program, BldBrIcc (Sec VI) to generate the direct access and index files and the interactive use of the BrIcc (Sec VII) and its use as an evaluation tool (Sec VII B and VII C).

II. GAMMA TRANSITIONS RECORDS

The GAMMA and the GAMMA continuation records, designed to hold the spectroscopic information on nuclear transitions, are particularly important to the BrIcc program. A short description of the fields of the **G** records (see Table II) is given in this section. The adopted procedures, relevant to BrIcc are described in Sec III.

A. GAMMA records

Transition energy (E) and uncertainty (DE) fields: The transition energy, **E** (E_γ) and the symmetric uncertainty, **DE** (ΔE_γ) are given in keV. In a relatively small cases, asymmetric uncertainty values are given in the GAMMA continuation record using the ENSDF dictionary term, DE= with two signed, maximum two digits integer numbers. For example, E=12.4, DE=+1-2 will correspond to a transition energy of $E = 12.4^{+0.1}_{-0.2}$ keV. The asymmetric uncertainties of E_γ will be referred as ΔE_H and ΔE_L.

Photon Intensity (RI) and uncertainty (DRI): The experimental photon intensity is given in the **RI** and in the **DRI** fields. The numerical values are I_γ and ΔI_γ. Pure E0 transitions are treated differently; here **RI** is blank but the total intensity, **TI**, is given (see below).

Multipolarity (M) field: can contain a maximum of 3 multipolarities, including E0,E1,E2,...E6,M1,M2,...M6 (corresponding to electric monopole, electric/magnetic dipole, etc) or D,Q,... (dipole, quadrupole, etc.). To mark assumed, doubtful, and mixed multipolarities the following characters are used [ ] ( ) + and ,(comma). Some typical combinations are listed in Table IV. In the case of mixed multipolarity the lowest two

multipole orders will be used by the program BrIcc to calculate the conversion coefficient. *E0+M1+E2* transitions are treated differently. The *M1* or *E2* multipolarity is considered first and the **E0** is considered last. If any non-standard character is present in the **M** field, the multipolarity (and mixing ratio) will be omitted.

Mixing Ratio (MR) field: The multipole mixing ratio, δ is defined as the ratio of two absolute transition amplitudes [1974AlAA]:

$$\delta(\pi'L'/\pi L) = \frac{\gamma(\pi'L')}{\gamma(\pi L)} \tag{1}$$

The + or - character in the **MR** field indicates that the sign of the mixing ratio is known.

In some cases three multipolarities can mix and in a similar way to Eqn. 1 one can define:

$$\delta(\pi''L''/\pi'L') = \frac{\gamma(\pi''L'')}{\gamma(\pi'L')}. \tag{2}$$

Valid combination of mixed multipolarities ($0 \leq L \leq 5$) include:

	$\Delta\pi = +1$			$\Delta\pi = -1$	
πL	M1	M1	M3	E1	E3
$\pi'L'$	E2	E2	E4	M2	M4
$\pi''L''$	M3	E0	M5	E3	E5

In the case of *E0+M1+E2* transitions the **MR** field is reserved for the $\delta(E2/M1)$ mixing ratio. The *E0,E2* mixing ratio,

$$q^2(E0/E2) = \frac{I_K(E0)}{I_K(E2)} \tag{3}$$

can be specified in the GAMMA continuation record as **MRKE0/E2**. *This term is yet to be defined in the ENSDF dictionary and manual.* Conversion coefficients for mixed multipolarity transitions with E0 component (M1+E2+E0, M1+E0, E2+E0, etc.) are calculated without the monopole contribution.

Similarly, mixed transitions with three multipole components of E1-E5, M1-M5 are treated as mixed transitions with two multipole components. The correct treatment of mixed transitions with three multipole or E0 component are planned in future release of BrIcc.

Mixing Ratio Uncertainty (DMR) field: A single integer or two integers with + and - signs in the **DMR** field will be interpreted as symmetric or asymmetric uncertainty values, respectively. In some cases the **DMR** field contains *GE, GT, LE, LT* or *AP* strings indicating a limit on **MR** or that **MR** is an approximation. Some examples of the coding and interpretation of the **MR** and **DMR** field are given in Table IV. The asymmetric uncertainties of δ are only indicated if **MR** has either a + or a - sign and will be referred as $\Delta\delta_H$ and $\Delta\delta_L$.

Total Conversion Coefficient (CC) and Uncertainty (DCC) fields: If the multipolarity and mixing ratio are known, the total conversion coefficient is calculated by the BrIcc program. Numerical value of **CC** and the symmetric uncertainty is labeled as α_{tot} and $\Delta\alpha_{tot}$. **CC** will be placed onto the new **G** record if $\alpha_{tot}/(1+\alpha_{tot}) \geq 10^{-4}$, otherwise it will be placed on the '**S G**' GAMMA continuation record. If **CC** is derived purely from theoretical conversion coefficient the **DCC** field should be left blank on the **G** record. See Sec. III for the calculation method used.

Relative Total Intensity (TI) and uncertainty (DTI) fields: If the photon intensity, I_γ, and the total conversion coefficient, α_{tot} are known, the relative total intensity, I_{tot} is defined as

$$I_{tot} = I_\gamma * (1 + \alpha_{tot}). \tag{4}$$

For pure *E0* transitions I_{tot} is the sum of electron conversion (I_K, I_{L1}, ...) and pair conversion I_{IPF} intensities. Higher order effects of electromagnetic transitions are usually neglected.

If the **TI** is given, values of the K/T, L/T, *etc.* theoretical shell to total intensity ratios, are placed in the **S G** records.

B. GAMMA continuation records

Table III gives the short description of the GAMMA continuation records. There are two basic type of GAMMA continuation records.

1. '2 G' GAMMA continuation records

Any character, other than 1 or S in column 6 can be used to create a GAMMA continuation record. This record is intended to store quantities (see Table III), which are not defined in the **G** record. Quantities which will be read in by BrIcc are marked in the Table. '**2 G**' records are created by the ENSDF evaluators.

2. 'S G' GAMMA continuation records

This type of record, with a character 'S' in column 6, is a special type of continuation record which flags the Nuclear Data Sheets production code to suppress the data contained on it for the publication. BrIcc generates '**S G**' records and the data on these records are used by other programs. Conversion coefficients and uncertainties are calculated as described in Sec. III. Electron to total intensity ratios are calculated from the conversion coefficients.

The BrIcc program will scan the '**S G**' records of the input ENSDF file. A warning message will be inserted into the calculation report file if any non-standard dictionary term

is found. The non-standard quantity will be placed on a new **'S G'**. See Table III for the list of dictionary terms expected in **'S G'** records. Please note that with the exception of RadList, none of the current ENSDF utility programs extract any numerical values from the **'S G'** records.

III. CALCULATION OF CONVERSION COEFFICIENTS

Electron conversion coefficients (α_K, α_{L1}, α_{L2}, ... etc.) and electron–positron pair conversion coefficient (α_{IPF}) are calculated by BrIcc. Values for pure multipolarity transitions are obtained by a cubic spline interpolation of the tabulated values (see sec V). Input parameters, atomic number Z, transition energy E_γ and multipolarity are obtained by the program from the **IDENTIFICATION** record: **DSID**; from the **GAMMA** record: **NUCID**, **E**, **DE**, **M**, **MR** and **DMR** fields of the **G** records. The program will verify the values obtained from the above fields and will generate warning and error messages to help resolve coding errors. As this function of the program is not designed to carry out full checking of the ENSDF file, the use of FmtChk, prior to use BrIcc is highly recommended.

In some of the following cases BrIcc will not generate new **G** or **S G** (ε_{ic} denotes the binding energy for the ic-subshell):

(a) $E_\gamma + \Delta E_H < \varepsilon_{ic}$ – no calculation for that subshell but new **G** and **S G** records are generated.

(b) $E_\gamma - \Delta E_L \leq \varepsilon_{ic} + 1$ keV – no calculation for that subshell and NO new **G** or **S G** records are generated.

(c) $Z < 10$ or $Z > 95$ (outside of the range of the tabulations) - no calculations and NO new **G** or **S G** records are generated.

(d) $E_\gamma - \Delta E_L > 6000$ keV, the energy range of the tabulations (see table I) – no calculation for that subshell and NO new **G** or **S G** records are generated.

(e) For some subshells (see sec V A) the energy range of the tabulations less than 6000 keV – no calculation for that subshell but new **G** and **S G** records are generated.

For mixed ($\pi L + \pi' L'$) multipolarity transitions the conversion coefficient can be obtained from the following formula:

$$\alpha = \frac{\alpha(\pi L) + \delta^2 \alpha(\pi' L')}{1 + \delta^2}, \tag{5}$$

where $\alpha(\pi L)$ and $\alpha(\pi' L')$ are the conversion coefficients for the pure multipolarities to be mixed.

The (symmetric) uncertainty of the conversion coefficient, $\Delta\alpha$, is made up of a number of contributions. In some cases $\Delta\alpha$ uncertainty is asymmetric. In this cases the larger absolute value should be adopted for the symmetric uncertainty.

$\Delta\alpha_{\mathbf{theo}}$ By comparing the electron conversion coefficients of Band et al., [2002Ba85] to experimental values, Raman et al., [2002Ra45] have concluded, that the accuracy of the theoretical α values is in the range of 0-1 %.

We have no knowledge of any information on the accuracy of the other data tables (α_{IPF}, $\Omega(E0)$) used by BrIcc.

Additional uncertainty may be associated to the cubic spline interpolation used in the same way for all data tables.

We adopted a relative uncertainty of 1.36% for the electron conversion and pair conversion coefficients deduced from the tables. The $\Delta\alpha_{theo}$ symmetric uncertainty incorporates both, the accuracy of the theoretical calculations and the accuracy of the interpolation. For further details see Sec V A.

$\Delta\alpha_{\mathbf{DE\_H}}$, $\Delta\alpha_{\mathbf{DE\_L}}$ The value of the conversion coefficient, α is obtained by interpolation at the nominal transition energy, E_γ. One can define the asymmetric uncertainties, $\Delta\alpha_{DE\_H}$ and $\Delta\alpha_{DE\_L}$, deduced from the differences in conversion coefficients obtained for E_γ, $E_\gamma + \Delta E_H$ and $E_\gamma - \Delta E_L$ energies. In the case when either $E_\gamma + \Delta E_H$ or $E_\gamma - \Delta E_L$ is outside of the energy range of the data tables, α values are calculated at the energy limit of the tabulation.

$$
\begin{aligned}
\Delta\alpha_{DE\_H} &= \alpha(E_\gamma + \Delta E_H) - \alpha(E_\gamma)\,, \\
\Delta\alpha_{DE\_L} &= \alpha(E_\gamma - \Delta E_L) - \alpha(E_\gamma)\,.
\end{aligned}
\tag{6}
$$

If **DE** is a limit, new '**S G**' record will not be generated. In some cases **E** is equal to **DE**, which will be interpreted as only a limit is known for the transition energy and no calculations will be made.

$\Delta\alpha_{\mathbf{DMR\_H}}$, $\Delta\alpha_{\mathbf{DMR\_L}}$ In the case of mixed transitions, the uncertainties in the mixing ratio, $\Delta\delta_H$ and $\Delta\delta_L$, also contribute to $\Delta\alpha$. Depending on content of **DM** and **DMR** fields, the conversion coefficient, α and the $\Delta\alpha_{DMR\_H}$ and $\Delta\alpha_{DMR\_L}$ uncertainties associated with **DMR**, are determined in one of the following ways.

DMR *is given as symmetric or asymmetric uncertainty.* The conversion coefficient, α is calculated using Eqn. 5 and the uncertainties can be obtained as:

$$
\begin{aligned}
\Delta\alpha_{DMR\_H} &= \frac{[\alpha(\pi L) + \delta_H^2 \alpha(\pi'L')]}{1 + \delta_H^2} - \frac{[\alpha(\pi L) + \delta^2 \alpha(\pi'L')]}{1 + \delta^2}\,, \\
\Delta\alpha_{DMR\_L} &= \frac{[\alpha(\pi L) + \delta_L^2 \alpha(\pi'L')]}{1 + \delta_L^2} - \frac{[\alpha(\pi L) + \delta^2 \alpha(\pi'L')]}{1 + \delta^2}\,,
\end{aligned}
\tag{7}
$$

where $\delta_H = \delta + \Delta\delta_H$ and $\delta_L = \delta - \Delta\delta_L$. For unsigned values of **DM** the program will adopt $\delta_L = Max(\delta - \Delta\delta_L, 0)$.

$\boldsymbol{\Delta\alpha_{\mathbf{DMR\_H}},}$ **DMR** *is a lower limit.*
$\boldsymbol{\Delta\alpha_{\mathbf{DMR\_L}}}$
Continued

$$\alpha = \left[\alpha(\pi'L') + \frac{\alpha(\pi L) + \delta^2\alpha(\pi'L')}{1+\delta^2}\right] \times 0.5\,,$$

$$\Delta\alpha_{DMR\_H} = \Delta\alpha_{DMR\_L} = \left|\alpha(\pi'L') - \frac{\alpha(\pi L) + \delta^2\alpha(\pi'L')}{1+\delta^2}\right| \times 0.5\,. \qquad (8)$$

In this case $\Delta\alpha_{DE\_H}$ and $\Delta\alpha_{DE\_L}$ are deduced from the differences in $\alpha(\pi L)$ and $\alpha(\pi'L')$, obtained for energies of E_γ, $E_\gamma + \Delta E_H$ and $E_\gamma - \Delta E_L$.

DMR *is an upper limit.*

$$\alpha = \left[\frac{\alpha(\pi L) + \delta^2\alpha(\pi'L')}{1+\delta^2} + \alpha(\pi L)\right] \times 0.5\,,$$

$$\Delta\alpha_{DMR\_H} = \Delta\alpha_{DMR\_L} = \left|\frac{\alpha(\pi L) + \delta^2\alpha(\pi'L')}{1+\delta^2} - \alpha(\pi L)\right| \times 0.5\,. \qquad (9)$$

In this case $\Delta\alpha_{DE\_H}$ and $\Delta\alpha_{DE\_L}$ are deduced from the differences in $\alpha(\pi L)$ and $\alpha(\pi'L')$, obtained for energies of E_γ, $E_\gamma + \Delta E_H$ and $E_\gamma - \Delta E_L$.

MR *is an approximate value or derived from systematics,* **DMR** *is empty, an approximate value ('AP'), derived from systematics ('SY'), or calculated ('CA')* The conversion coefficient, α is calculated using Eqn. 5 and $\Delta\alpha_{DMR\_H} = \Delta\alpha_{DMR\_L} = 0$. **DCC** field is set to **DMR** if it is not empty ('AP', 'SY', or 'CA').

No **MR** *is given.* For cases when $L \neq L'$ (for example M1+E2 or M1,E2) δ is set to 1.

$$\alpha = [\alpha(\pi L) + \alpha(\pi'L')] \times 0.5\,,$$

$$\Delta\alpha_{DMR\_H} = \Delta\alpha_{DMR\_L} = |\alpha(\pi L) - \alpha(\pi'L')| \times 0.5\,. \qquad (10)$$

M *valid, but not unique multipolarity and* $L \equiv L'$ **(for example M1,E1).** α and $\Delta\alpha$ are calculated using Eqn 10.

M *contains dipole (D), quadrupole (Q), octupole (O), and their combinations.* No α or $\Delta\alpha$ are calculated and no new **'G'** or **'S G'** card will be generated.

A special case when the transition energy E *is an approximate value.* **DE** *is empty, an approximate value ('AP'), derived from systematics ('SY'), or calculated ('CA').* The conversion coefficient, α is calculated using Eqn. 5 and $\Delta\alpha_{DMR\_H} = \Delta\alpha_{DMR\_L} = 0$. **DCC** field is set to **DE** if is not empty ('AP', 'SY', or 'CA').

Combining the $\Delta\alpha_{theo}$, $\Delta\alpha_{DE\_H}$, $\Delta\alpha_{DE\_L}$, $\Delta\alpha_{DMR\_H}$ and $\Delta\alpha_{DMR\_L}$ partial values the

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symmetric uncertainty of the conversion coefficient is given as:

$$\Delta\alpha = \sqrt{(\Delta\alpha_{theo})^2 + (\Delta\alpha_{DE})^2 + (\Delta\alpha_{DMR})^2} \tag{11}$$

where

$$\begin{aligned} \Delta\alpha_{DE} &= Max(|\Delta\alpha_{DE\_H}|, |\Delta\alpha_{DE\_L}|) \\ \Delta\alpha_{DMR} &= Max(|\Delta\alpha_{DMR\_H}|, |\Delta\alpha_{DMR\_L}|)\,. \end{aligned} \tag{12}$$

The **DCC** field of the new **GAMMA** record will be blank if the contribution of the $\Delta\alpha_{DE\_H}$, $\Delta\alpha_{DE\_L}$, $\Delta\alpha_{DMR\_H}$ and $\Delta\alpha_{DMR\_L}$ terms are insignificant compare to the $\Delta\alpha_{theo}$ term.

If the total conversion coefficient, $\alpha_{tot} \geq 10^{-4}$, then it will be inserted into the **CC** field of the **G** record.

The program BRICC will generate **'S G'** continuation records if the conversion coefficient can be calculated. If $\alpha_{tot} < 10^{-4}$, α_{tot} and $\Delta\alpha_{tot}$ will be put on the first **'S G'** continuation record. BRICC will append further quantities onto the **'S G'** record(s). If the total intensity field, **TI** on the **G** record is empty (i.e. I_{tot} is not given) the conversion coefficient for the major shells, α_K, α_L, α_M and α_{N+} will be listed. (α_{N+} is the sum of the α_N, α_O, α_P, α_Q, α_R and α_{IPF} conversion coefficients.) Additional **'S G'** continuation record(s) will be created to list the α_N, α_O, α_P, α_Q, α_R and α_{IPF} conversion coefficients individually.

If the total intensity, I_{tot}, **TI** is given, instead of the conversion coefficients, BrIcc will append to the first **S G** continuation record the I_K/I_{tot}, I_L/I_{tot}, I_M/I_{tot} and I_{N+}/I_{tot} intensity ratios. Additional **'S G'** continuation record(s) will be generated for intensity ratios involving the N, O, P, Q, R and S shells and electron–positron pair production. For example for the K-shell we get:

$$\frac{I_K}{I_{tot}} = \frac{\alpha_K}{1 + \alpha_{tot}}. \tag{13}$$

There is some covariance, for example between α_K and α_{tot}, which can be taken into account in the following way. Let us define the ratio, x as

$$x = \frac{a}{a + b}. \tag{14}$$

The uncertainty, Δx can be expressed as:

$$\Delta x = \frac{\sqrt{(\Delta a \times b)^2 + (a \times \Delta b)^2}}{(a + b)^2}. \tag{15}$$

Considering a case when nuclear transition involves the emission of gamma–rays and internal conversion *via* K–, L– and M–shells, to evaluate the I_K/I_{tot} we get $a = \alpha_K$ and $b = 1 + \alpha_L + \alpha_M$.

IV.   CALCULATION OF E0 ELECTRONIC FACTORS

Electric monopole (E0) transitions are possible between states of the same spin and parity in a nucleus enclosed by electrons. In 1987 Firestone [1987FiAA] outlined procedures for the evaluation of E0 transition probabilities for $0^+ \to 0^+$ monopole transitions, with particular emphasis on the Wilkinson estimates of single–particle transition probabilities. There has since been much activity in the field, both theoretical and experimental; see, for example, the recent review of Kibédi and Spear [2005Ki02].

The electric monopole operator couples the nucleus to the atomic electrons, giving rise to the internal conversion process. It also couples the nucleus to the Dirac background to produce electron-positron pairs if the E0 transition energy is greater then twice the electron rest mass. Simultaneous emission of two photons is a higher order process (relative probability $\sim 10^{-3}$ to $\sim 10^{-4}$ [1986Vo07]) and for practical purposes can be neglected. Single–photon E0 transitions are strictly forbidden by considerations of angular-momentum conservation.

Here we outline the procedures relevant to evaluate pure electric monopole, E0 transitions. As it was indicated earlier (see sec. II), the procedures and the extension of BrIcc to handle mixed *E0+M1+E2* transitions is yet to be developed.

The E0 transition probability is given by the expression

$$W(E0) = \frac{1}{\tau(E0)} = W_{ic}(E0) + W_\pi(E0), \qquad (16)$$

where $\tau(E0)$ is the partial mean life of the initial state for E0 decay. The quantities $W_{ic}(E0)$ and $W_\pi(E0)$ are the transition probabilities for internal–conversion electron and electron-positron pair emission, respectively. They are given by the expression

$$W_{ic}(E0) + W_\pi(E0) = \rho^2(E0) \times [\Omega_{ic}(E0) + \Omega_\pi(E0)], \qquad (17)$$

where $\Omega_{ic}(E0)$ and $\Omega_\pi(E0)$ are electronic factors defined by Church and Weneser [1956Ch21]. They are functions of atomic number, Z, and transition energy. They can be calculated independently of nuclear properties. The quantity $\rho(E0)$ is the dimensionless monopole transition strength. It carries all the information about the nuclear structure, being related to the monopole matrix element according to the expression

$$\rho(E0) = \frac{< f|M(E0)|i >}{eR^2}, \qquad (18)$$

where R is the nuclear radius. It is usually assumed that $R = r_\circ A^{1/3}$, where A is the atomic mass number and $r_\circ = 1.20$ fm.

The reduced E0 transition probability $B(E0)$ is equal to the square of the E0 matrix element, and so

$$B(E0) = \rho^2(E0)e^2R^4, \qquad (19)$$

where e is the electronic charge. Clearly $\rho(E0)$ is a basic characteristic of electric monopole transitions. Because there is often an ambiguity in determining its sign, it is customary to

use $\rho^2(E0)$. Since the value of $\rho^2(E0)$ usually lies in the range 10^{-3} to 10^{-1}, reference is usually made to $10^3\rho^2(E0)$. It is evident from equation (17) that experimental determination of $\rho^2(E0)$ requires the measurement of absolute transition rates and the calculation of electronic factors. In some cases the transition rate can be determined indirectly from that of another transition de-exciting the same nuclear state, provided that the relevant branching ratio is known.

In their discussion of E0 transitions between 2^+ states, Church, Rose and Weneser [1958Ch48] introduced the quantity

$$q_K^2(E0/E2) = \frac{I_K(E0)}{I_K(E2)}, \tag{20}$$

where $I_K(E0)$ and $I_K(E2)$ represent the intensities of E0 and E2 K-conversion electron components of the $J_i^+ \to J_f^+$ transition, respectively.

The definition of $q_K^2(E0/E2)$ can be extended to the case of $0_i^+ \to 0_f^+$ transitions (which can have no E2 component) by somewhat arbitrary reference to an E2 transition from the 0_i^+ state to a 2_f^+ state [1972Al57, 1974Ha63, 1994Ki01]. Usually this is taken to be the first excited 2^+ state (2_1^+).

In some cases experimental information other than $I_K(E0)$ and $I_K(E2)$ can be used in conjunction with the relevant conversion coefficients and electronic factors to deduce $q_K^2(E0/E2)$. For example,

$$q_K^2(E0/E2) = \frac{I_\pi(E0)}{I_\pi(E2)} \times \frac{\Omega_K(E0)}{\Omega_\pi(E0)} \times \frac{\alpha_\pi(E2)}{\alpha_K(E2)}, \tag{21}$$

where $I_\pi(E0)$ and $I_\pi(E2)$ are the observed internal pair intensities for the E0 and E2 transitions, respectively, and $\Omega_{K,\pi}(E0)$ and $\alpha_{K,\pi}(E2)$ are the relevant electronic factors and conversion coefficients.

A dimensionless ratio of the E0 and E2 reduced transition probabilities was defined by Rasmussen [1960RaAA]:

$$X(E0/E2) \equiv \frac{B(E0)}{B(E2)} = \rho^2(E0)e^2R^4/B(E2). \tag{22}$$

The equivalent experimental value, considering K conversion electrons, can be deduced from the general formula:

$$X(E0/E2) = 2.54 \times 10^9 A^{4/3} \times q_K^2(E0/E2) \times \frac{\alpha_K(E2)}{\Omega_K(E0)} \times E_\gamma^5, \tag{23}$$

where E_γ is the E2 γ-ray energy in MeV.

The experimental monopole strength can be obtained directly if the partial mean life of the E0 transition, $\tau(E0)$, is known

$$\rho^2(E0) = \frac{1}{[\Omega_K(E0) + \Omega_{L1}(E0) + ...\Omega_\pi(E0)] \times \tau(E0)}. \tag{24}$$

Alternatively, if the E2 transition rate, $W_\gamma(E2)$, is known, $\rho^2(E0)$ can be obtained from the expression

$$\rho^2(E0) = q_K^2(E0/E2) \times \frac{\alpha_K(E2)}{\Omega_K(E0)} \times W_\gamma(E2). \qquad (25)$$

For pure electric monopole (E0) transitions the $\Omega_K(E0)$, $\Omega_{L1}(E0)$, $\Omega_{L2}(E0)$ and $\Omega_{IPF}(E0)$ electronic factors are calculated and listed in the BrIcc report file. The accuracy of the calculated $\Omega(E0)$ values is believed to be better than 5%. The current version of BrIcc does not assign any uncertainty to the interpolated values. Part of the BrIcc calculation report file of an E0 transition is shown in Fig. 1.

FIG. 1: BrIcc calculation report for an E0 transition.

```
=================================================================================================
BrIcc v2.0 (22-Sep-2005)  Z= 40  Egamma= 1487.5 1 keV          Multipolarity= E0                22-SEP-05

Shell   Omega(E0)
        ---------
K      1.719E+09
L1     1.812E+08
L2     1.405E+06
IPF    1.875E+08
Tot    2.090E+09

K/Tot 8.229E-01

 Compare OLD/NEW cards
   141 :  90ZR  G 1487.5    1 1.9     6 E0                                            <Old Card Kept>
```

V. DATA TABLES

The data tables, large ASCII files, have been assembled from various printed tables and electronic files. The electron conversion coefficient table (see next section) has been calculated specifically for BrIcc. The various ASCII files are converted into a single binary file (BrIccFO.icc) for quick computer access. The main features of the data tables are summarized in Table I. An additional binary file (BrIccFO.idx) contains the location of all $\alpha_i(Z)$ and $\Omega_i(E0, Z)$ data sets.

NOTE: The ScPcc, HoPcc, HsOmg, BeOmg and PaOmg data tables were produced from printed material, using a scanner and character recognition software, they may contain errors. Please report them to the authors for correction.

A. Dirac-Fock Internal Conversion Electron Coefficients (BrIccFO)

The conversion electron coefficient tables based on the model developed by Band *et al.*, [2002Ba85]. The original table, published in 2002, was calculated using the so–called *'No Hole'* approximation and had an energy range of $\epsilon_{L1} + 1$ keV to 2000 keV, covering all atomic shells in Z=10 to 126 elements. The first development version of BrIcc was based

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TABLE I: Theoretical tabulations of internal conversion coefficients and electronic factors used by BrIcc.

Data Table	Reference	Z	Shells or IPF	L	E_γ [keV][a]
Internal conversion coefficient α_{ic} using the 'Frozen Orbital' approximation					
BrIccFO	This work based on the model of [2002Ba85, 2002Ra45]	10–95	All shells	1–5	ε_{ic}+1–6000
Pair conversion coefficient α_{IPF}					
ScPcc	[1979Sc31]	0–100[b]	IPF	1–3	1100–8000
HoPcc	[1996Ho21]	50–100	IPF	1–3	1100–8000
Electronic factor Ω(E0)					
HsOmg	[1969Ha61]	30–42	K^c, L_1^d, L_2^d	0	ε_K+6–1500
BeOmg	[1970Be87]	40–102	K	0	51^e–2555
		40–102	L_1, L_2	0	51–2555
PaOmg	[1986PaZM]	8–40	K^d	0	511–12775
		8–40	IPF	0	1430.8–12775

[a] ε_{ic} is the binding energy for the ic–shell.

[b]   Used for $Z < 50$

[c]   Not used

[d]   Used for $Z < 40$

[e]   For Z=40–58: 51.1 keV; for Z=60–82: 102.2 keV; for Z=84–96: 153.3 keV
and for Z=98–102: 204.4 keV

on the same physical model. However, some modifications of the original *RAINE* program were required to extend the energy range to 6000 keV and increase the numerical accuracy of the calculations for some cases, e.g., M4–shell for Z=23, N4 and O4 for Z=21, 58, 64, *etc.* It was also noted that for certain outer shells (N6-shell for Z=59–75, and N7-shell for Z=63–75), the calculated conversion coefficients are non–monotonous values oscillating as a function of transition energy. It was assumed, that this it caused by limitation in the numerical methods used in the program. For these cases, the range of the tabulations has been reduced to about 400. It should be noted that for 400 keV transition energy in Z=59 (Praseodymium) the $\alpha_{N6}(E2)$ conversion coefficient is about 10^{-9} times smaller than the total conversion coefficient. Neglecting these shells from the evaluation of the **CC** has little or no effect.

An important question, discussed several times in the past decades, is the overall accuracy of the theoretical conversion coefficients, see for example Raman *et al.* [2002Ra45] and references therein. To answer the question, *'How good are the internal conversion coefficients now?'*, Raman *et al.* assembled a list of 100 experimental α_K and α_T conversion coefficients known to better than 5% accuracy. By comparing experiment to various theoretical values, Raman *et al.* [2002Ra45] concluded, that the best agreement with experiment can be achieved with the new Dirac-Fock model [2002Ba85] and without taking into account the effect of the atomic vacancy. Since then, an important development was the

determination of the α_K conversion coefficient of the 80.236 (7) keV M4 transition in the 10.5 day isomer decay in ^{193}Ir by Nica *et al.* [2004Ni14]. The new results clearly demonstrate that the effect of the atomic vacancies should not be neglected in the theoretical calculations.

The BrIccFO data table presented here is based on the so–called *'Frozen Orbital'* approximation, which takes into account of the effect of the atomic vacancy (hole) created during the conversion process [2002Ra45]. In this approximation the bound wave functions are calculated in the self–consistent field of a neutral atom and the continuum wave functions are calculated in an ion field constructed from bound wave functions of a neutral atom. This version of the BrIccFO data table covers Z=10 to 95 elements. In future release of the program it is planned to cover heavier elements.
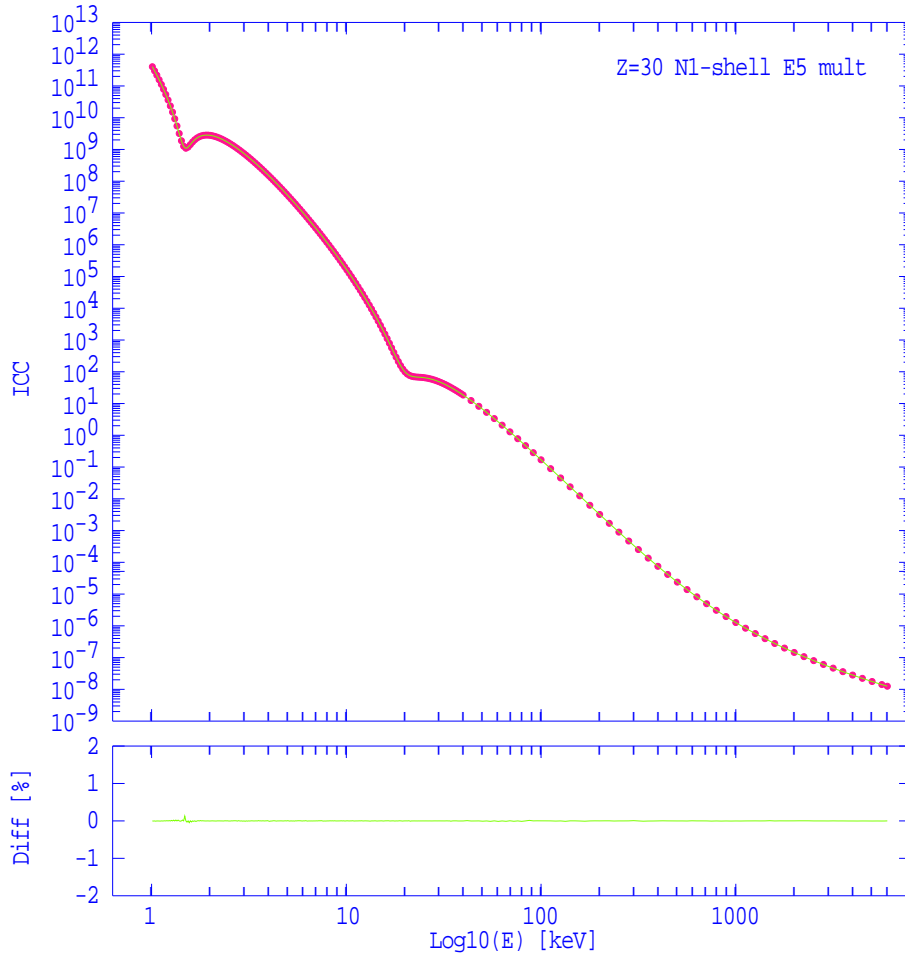

FIG. 2: E5 conversion coefficients for the N1–shell in ^{64}Zn in the 'resonance'–like region. Top panel compares the calculated values (open circles, current work and [2006KiAA]) with values obtained using cubic spline interpolation (solid curve). Bottom panel shows the differences between interpolated and directly calculated values in percentage. See text for further explanation.

Representative conversion coefficients are shown in Fig. 2. For lighter element it was suggested [2002Ba85, 2002Ra45], that the conversion coefficient for some of the $s_{1/2}$ shells

are not monotonous. It was attributed to cancelation effects of the leading matrix elements causing sharp reduction of the conversion coefficient. This so–called 'resonance'–like effect is clearly visible on Fig. 2 at 20 keV transition energy for $\alpha_{N1}(E5)$ in ^{64}Zn. Similar features can be observed for E3-E5 multipolarities for most of the lighter elements. Another type of irregularities is emerging on Fig. 2 at very low energies. This is a threshold irregularity effect and is assumed to be different in character. Both effects have been explored further in order to establish empirical relation between the position of the irregularity (the transition energy, where the conversion coefficient take the minimum value) and the atomic number Z [2005KiZW]. Fig. 3 shows the results together with the proposed empirical relations.
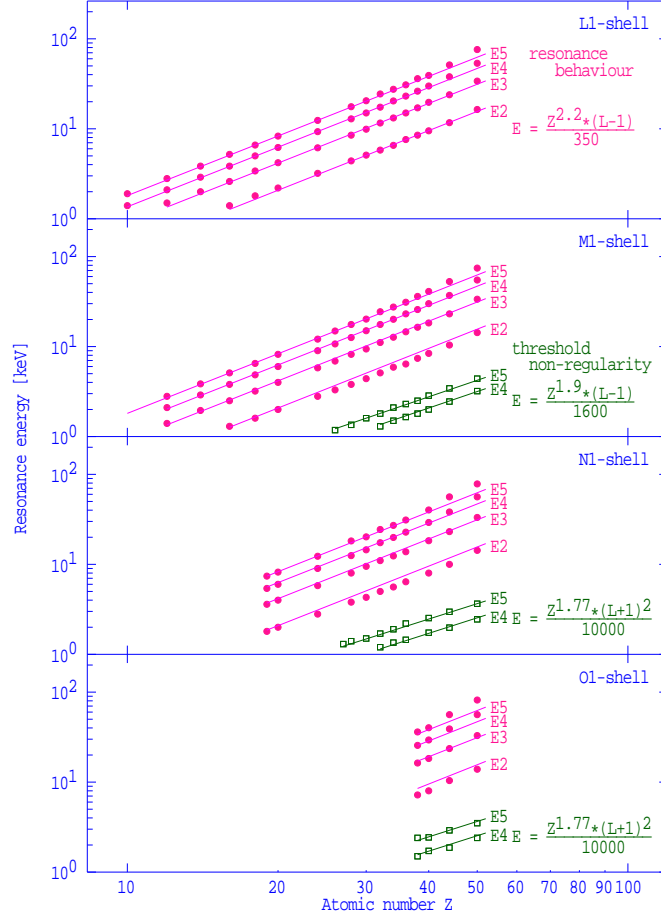

FIG. 3: Position of the 'resonance'– and threshold non–regularity regions as a function of atomic number of Z. Note the logarithmic scale on both axes. Approximate relations are also displayed.

Extra care was taken to increase the accuracy of the interpolation procedure [2005BuAA], especially in the above mentioned resonance regions. To evaluate the difference between the directly calculated and the interpolated values, we have used the

$$\Delta ICC(set1 : set2) = \frac{ICC(set1) - ICC(set2)}{ICC(set2)} \times 100 \tag{26}$$

quantity, which gives the percentage difference between two values of set1 and set2. The bottom panel of fig. 2 shows the $\Delta ICC(Int : Calc)$ difference between interpolated (Int) and calculated (Calc) values. The difference was evaluated at the mesh points and at the middle between two mesh points for the range of the table. (Calculated values were obtained using the RAINE code for specific energies.) Evaluating the average value of $\Delta ICC(Int : Calc)$ differences over a wide range of atomic numbers, sub–shells and multipolarities, let us to establish an upper limit 0.3 % for the numerical accuracy of the interpolation procedure. It was noted that in some cases, interpolated values obtained on different computer platforms (Windows, Linux or UNIX) may be different. Closer look of the problem revealed, that the relative differences are usually at the level of $< 0.2\%$. The elimination of this problem will be one of the important improvements for future release of the program.

We have adopted the basic principles of the work [2002Ra45] to compare the calculated conversion coefficient to experimental data. In the course of this review we have re-examined the available experimental data and made several adjustments to the adopted values of high precision conversion coefficients. The present list contains about 140 α_K, α_L, $\alpha_{K/L}$ and α_T values. Comparing the experimental ICC's to the *'Frozen Orbital'* approximation gives an average difference $\Delta ICC(Exp : Frozen\,Orbital)$ of $-1.01(21)$ %, which is a lower value than previously adopted. The similar comparison to the so-called *'No Hole'* approximation gives a value of $\Delta ICC(Exp : No\,Hole) = +0.58(28)$ %, which is slightly higher than cited in [2002Ra45]. In the latter case, it is important to note, that the average difference for the K-shell (comprises about 50 % of the data), $\Delta ICC(Exp : No\,Hole) = +1.8(5)$ % and $\Delta ICC(Exp : Frozen\,Orbital) = 0.73(35)$ %. The recent meeting of international Nuclear Structure and Decay Data Network, held in June 2005 adopted the *'Frozen Orbital'* approximation for the calculated conversion coefficients for use in ENSDF evaluations.

Based on the above average differences of $0.0(3)$ % between calculated and interpolated values, and $-1.01(21)$ % between calculated and experimental values, we have estimated a 1.4 % symmetric uncertainty ($\Delta\alpha_{theo}$) for the accuracy for BrIccFO conversion coefficients.

B. Conversion Coefficients for Electron-Positron Pairs (ScPcc and HoPcc)

Two data sets, ScPcc for $Z < 50$ [1979Sc31] and HoPcc for $Z \geq 50$ [1996Ho21] have been assembled using the printed tables. The latter calculation takes into account the effect of the finite size of the nucleus, which is expected to be a sizable ($> 1\%$) effect in the $Z \geq 50$ elements.

The original tabulations were given up to three valuable digits and for Z=0, 10, 20, ...100 atomic numbers and energies ranging from 1100 keV to 8000 keV. To obtain $\alpha_\pi(E_\gamma, Z, \pi L)$, the pair conversion coefficient, two dimensional interpolation has to be used over the (Z, E_γ) plane. To simplify the numerical calculations, the first step, the interpolation over Z has been carried out as part of the procedure to assemble the binary data file, *BrIccFO.icc*. Typical electron positron pair conversion coefficients in Ytterbium (Z=70) are shown in Fig. 4. We have assumed the same value of 1.4 % for the $\Delta\alpha_{theo}$.
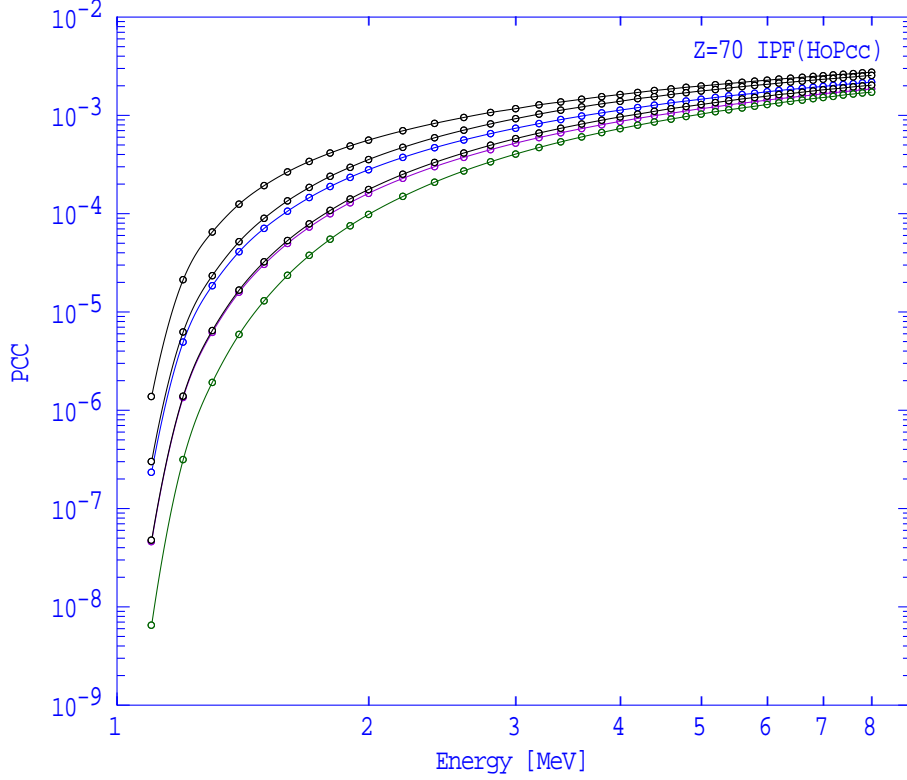
FIG. 4: Electron–positron pair conversion coefficients (α_π or PCC) in Yb. Tabulated values (open circles) taken from [1996Ho21] are compared with values obtained using cubic spline interpolation (solid curves).

C.   Electronic factors for E0 transitions (HsOmg, BeOmg and PaOmg)

Three different tabulations, listed below, are partially overlapping in terms of atomic number Z, transition energy. The subset of data included in the conversion data base is indicated in each case. The original printed tables were digitized using an optical scanner and character recognition software. Please report any errors to the authors for correction.

(a) Data set label: `HsOmg`
Reference: 1969Ha61 [1969Ha61]
Z-range: 30,34,38,42 (original table). Intermediate values for Z=32,36,40 were obtained by cubic spline interpolation.

Tabulated values of $A(E0, Z, k)$ have been converted to $\Omega(Z, k)$ using the following formulae:
$\Omega(Z, k) = \frac{8\pi m_\circ c^2}{\hbar} A(E0, Z, k)k.$

Energy range: K-shell: 15.9(26.2)-1500 keV, L1-Shell: 7.4(9.1)-1500 keV, L2-shell: 7.2(8.8)-1500 keV
Electron shells: K, L1, L2
BrIcc data base includes: L1 and L2 shells and Z=30,32,..38.

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(b) Data set label: BeOmg
   Reference: 1970Be87 [1970Be87]
   Z-range: 40,42,44,...102
   Energy range: 51.1-2555.0 keV
   Electron shells: K, L1, L2
   BrIcc data base includes: all data

(c) Data set label: PaOmg
   Reference: 1986PaZM [1986PaZM]
   Z-range: 8,10,12,...40
   Energy range: 511-12775 keV (K-shell); 1430.8-12775 (IPF)
   Electron shells: K, IPF (BrIcc treats IPF coefficients in the same way as the electron shells.)
   BrIcc data base includes: all data, except K-shell for Z=40

VI.   BLDBRICC PROGRAM

This program reads the BldBrIcc.dat file, which contains the file names of the ASCII data files, listed in the previous chapter. It requires the 'BrIccHome' environment variable to be set to locate the data files on the various platforms (see sec IX).

BldBrIcc.dat: (input) Contains the home directory of BrIcc and the file names of the ASCII data files, listed in the previous chapter.

BRICC.IDX: (output) The ICC index file containing 2048–bytes records for elements from Z=1 to 126. Each record contains the atomic number, the atomic mass used to calculate the conversion coefficient, the chemical symbol and the first record number in the BRICC.ICC file where any of the 41 'shells' (α_K, α_{L1}, ... α_{R2}, α_{total}, α_{IPF}, Ω_K, Ω_{L1}, Ω_{L2} and Ω_{IPF}) is starting. The record number is set to zero if no data are available for that shell.

BRICC.ICC: (output) The ICC data file. Each record is 44 bytes long and contains the transition energy and a maximum of 10 conversion coefficients (E1-E5,M1-M5) or just a single electronic factor.

Terminal dialog: The program will look for and open the input file. The program will report if the sequential data files were successfully opened and will report the progress (see Fig 5).

VII.   BRICC PROGRAM

This program calculates the internal conversion electron and electron-positron pair coefficients and electronic factors for E0 transitions by cubic spline interpolation on the Log-Log

```
BldBrIcc v2.0 22-Sep-2005 creating BrIccFO.idx and BrIccFO.icc files
--------------------------------------------------------------------------------
Data sets to process:
BrIccFO   \Data\BrIccFO\BrIccFO.txt
Pcc       \Data\Pcc\Pcc.txt
HsOmg     \Data\HsOmg\HsOmg.txt
BeOmg     \Data\BeOmg\BeOmg.txt
PaOmg     \Data\PaOmg\PaOmg.txt
--------------------------------------------------------------------------------
Processing data:
Created lookup file: BrIccFO.idx
Created direct access data file: BrIccFO.icc
DataSet    Z Shell   Record
--------------------------------------------------------------------------------
ScPcc      1 IPF         1
ScPcc      2 IPF        41
...
...
ScPcc      8 IPF       281
PaOmg      8 K         321
PaOmg      8 IPF       412
ScPcc      9 IPF       485
BrIccFO   10 K         525
BrIccFO   10 L1        624
BrIccFO   10 L2        796
BrIccFO   10 L3        883
ScPcc     10 IPF       970
PaOmg     10 K        1010
PaOmg     10 IPF      1101
...
...
--------------------------------------------------------------------------------
BrIccFO.idx and BrIccFO.icc files were created
```

FIG. 5: BLDBRICC terminal dialog.

scale.

'BrIccHome': The home directory of the program is defined by setting the value of the 'BrIccHome' environment variable to point to the dirrectory, where the program is located. (See section IX for further details.)

Input files: Data files, created by BLDBRICC, are
%BrIccHome%\BrIcc.idx (ICC index file)
and
%BrIccHome%\BrIcc.icc (binary file of ICC's).

Terminal dialog: The BRICC program can be used in three different ways: (a) interactively to calculate ICC, (b) to generate GAMMA and SG records for an ENSDF file, (c) insert (merge) newly created records with existing ENSDF file.

A. BRICC – interactive use

Program execution: `BRICC<CR>`. It will invoke the program with default values of Z=70 (Ytterbium) and E_γ=279.717 keV.

Terminal dialog: The program uses 116 characters lines to report conversion coefficient for E1-E5 and M1-M5 multipolarities, see Fig. 6. Consult with the documentation of the operating system used to set the width of the terminal window accordingly. A list of interpolated conversion coefficients for all major and subshells, for electron–positron pair creation, etc.

```
-------------------------------------------------------------------------------------------------------
Z= 70  Ytterbium        Transition energy: 279.717 keV                        BrIcc v2.0 (22-Sep-2005)
                                                Conversion Coefficient
Shell  E_e [keV]   E1       M1        E2        M2        E3        M3        E4        M4        E5        M5
-------------------------------------------------------------------------------------------------------
Tot              2.367E-02 1.900E-01 9.150E-02 8.109E-01 4.258E-01 3.015E+00 2.266E+00 1.179E+01 1.250E+01 4.966E+01
K       218.38   1.989E-02 1.593E-01 6.401E-02 6.436E-01 1.910E-01 2.138E+00 5.694E-01 6.978E+00 1.740E+00 2.279E+01
L1      269.23   2.342E-03 2.191E-02 7.477E-03 1.080E-01 2.580E-02 4.547E-01 1.063E-01 1.900E+00 5.021E-01 7.981E+00
L2      269.74   3.016E-04 1.784E-03 8.317E-03 1.356E-02 1.018E-01 8.394E-02 8.120E-01 4.715E-01 5.323E+00 2.502E+00
L3      270.77   3.027E-04 2.329E-04 5.354E-03 7.571E-03 5.104E-02 1.308E-01 3.609E-01 1.249E+00 2.193E+00 9.463E+00
L-tot            2.946E-03 2.393E-02 2.115E-02 1.292E-01 1.787E-01 6.694E-01 1.279E+00 3.621E+00 8.019E+00 1.995E+01
M1      277.32   5.074E-04 4.853E-03 1.631E-03 2.463E-02 5.883E-03 1.073E-01 2.603E-02 4.644E-01 1.315E-01 2.021E+00
M2      277.54   7.192E-05 4.375E-04 2.036E-03 3.373E-03 2.540E-02 2.121E-02 2.063E-01 1.212E-01 1.377E+00 6.544E-01
M3      277.77   7.427E-05 5.792E-05 1.351E-03 1.949E-03 1.305E-02 3.462E-02 9.310E-02 3.405E-01 5.708E-01 2.657E+00
M4      278.14   1.112E-06 1.001E-06 1.102E-05 2.250E-05 1.503E-04 4.745E-04 4.054E-03 6.278E-03 6.572E-02 6.348E-02
M5      278.19   1.402E-06 8.146E-07 8.490E-06 3.852E-06 1.411E-04 1.213E-04 2.812E-04 4.201E-04 3.712E-02 7.142E-02
M-tot            6.561E-04 5.350E-03 5.038E-03 2.998E-02 4.462E-02 1.637E-01 3.323E-01 9.366E-01 2.182E+00 5.467E+00
N1      279.23   1.189E-04 1.143E-03 3.828E-04 5.840E-03 1.396E-03 2.563E-02 6.279E-03 1.118E-01 3.220E-02 4.906E-01
N2      279.32   1.635E-05 1.001E-04 4.657E-04 7.740E-04 5.834E-03 4.885E-03 4.756E-02 2.802E-02 3.188E-01 1.519E-01
N3      279.37   1.681E-05 1.315E-05 3.078E-04 4.457E-04 2.980E-03 7.969E-03 2.131E-02 7.890E-02 1.309E-01 6.196E-01
N4      279.52   2.574E-07 2.325E-07 2.559E-06 5.253E-06 3.504E-05 1.113E-04 9.507E-04 1.477E-03 1.548E-02 1.500E-02
N5      279.53   3.210E-07 1.869E-07 1.943E-06 8.836E-07 3.261E-05 2.817E-05 6.539E-04 9.822E-04 8.661E-03 1.679E-02
N6      279.71   3.233E-10 2.056E-10 1.991E-09 1.278E-09 1.744E-08 2.538E-08 2.017E-07 8.971E-07 7.373E-06 1.962E-05
N7      279.71   4.682E-10 2.459E-10 2.462E-09 1.035E-09 1.377E-08 5.023E-09 2.040E-07 1.316E-07 6.438E-06 7.161E-06
N-tot            1.526E-04 1.256E-03 1.161E-03 7.066E-03 1.028E-02 3.862E-02 7.675E-02 2.212E-01 5.060E-01 1.294E+00
O1      279.66   1.731E-05 1.666E-04 5.576E-05 8.525E-04 2.038E-04 3.747E-03 9.200E-04 1.638E-02 4.733E-03 7.198E-02
O2      279.69   1.934E-06 1.185E-05 5.514E-05 9.170E-05 6.913E-04 5.790E-04 5.638E-03 3.324E-03 3.783E-02 1.803E-02
O3      279.70   1.846E-06 1.445E-06 3.383E-05 4.904E-05 3.277E-04 8.777E-04 2.344E-03 8.701E-03 1.440E-02 6.841E-02
O-tot            2.109E-05 1.799E-04 1.447E-04 9.932E-04 1.223E-03 5.204E-03 8.902E-03 2.840E-02 5.696E-02 1.584E-01
P1      279.71   1.001E-06 9.637E-06 3.226E-06 4.932E-05 1.179E-05 2.169E-04 5.325E-05 9.479E-04 2.740E-04 4.167E-03
P-tot            1.001E-06 9.637E-06 3.226E-06 4.932E-05 1.179E-05 2.169E-04 5.325E-05 9.479E-04 2.740E-04 4.167E-03
Electronic Factor  E0
K       218.38 3.961E+10
L1      269.23 5.964E+09
L2      269.74 8.377E+07
TranEner | ChemSymb(2 char) | Z+IntValue | SUBShell | ? for help | EXIT [279.717] >
```

FIG. 6: BRICC interactive terminal dialog.

Parameter input:

Chemical symbol: Maximum of 2 characters. BrIcc will load the appropriate data set from disk.

Atomic number: Character Z followed by an integer, between 1 and 102 will be interpreted as an atomic number. BrIcc will load the appropriate data set from disk.

Transition energy: A positive number in free format, in keV. For example: 124, 124.0, 1.24E+2.

SUBShell: Will enable or disable the list of subshell ratios.

EXIT: Terminates the program execution.

Error handling: The program will reject an input string, which could not be interpreted as transition energy, chemical symbol, atomic number or subshell toggle on/off.

B. BRICC – ENSDF evaluation tool

Program execution: `BRICC` *ENSDF-file*`<CR>`.

The *ENSDF* file name is passed as program argument. A typical terminal dialog can be seen in Fig. 7.

WARNING: The input *ENSDF* file should not be modified before running the code in the MERGE mode (see sec. VII C).

NOTE: Set the working directory (path) on the Command prompt (Windows) or on the Console (Linux/UNIX) to the directory where the *ENSDF* file is. This will allow one to have all input and output files in the same directory.

Output files:

Calculation report: Complete report of calculations. Default file: *BRICC.LST*.

New G/SG records: New G/2 G records generated by the program, followed by the record number in the ENSDF input file. This is used as input to the program running as a utility to MERGE records. Default file: *CARDS.NEW*.

G/SG (New/Old) comparison report: Comparison of new and old G/2 G records. Default file: *COMPAR.LST*.

Execution control:

List conversion coefficients for all subshells (Def. N): The default is to only list the total conversion coefficients for the shell. Answering Yes (Y) will list all the subshell conversion coefficients in addition to the totals. Note that for higher atomic numbers this may be a very extensive list.

```
bricc BA1978Bo18.ens<CR>
         BrIcc v2.0 (22-Sep-2005) calculates conversion coefficients
                (for electron conversion and pair production)
                        and E0 electronic factors
                     using cubic spline interpolation
           Theoretical Dirac-Fock conversion coefficients based on
                the so-called "Frozen Orbital" approximation

 Input & Data Files:
    Index file: C:\Program Files\BrIcc\BrIccFO.idx
    ICC file: C:\Program Files\BrIcc\BrIccFO.icc
    Input ENSDF file: BA1978Bo18.ens

 Output Files:
    Complete calculations report, (Def: BrIcc.lst):
    New G/SG records, (Def: Cards.new):
    G/SG (New/Old) comparison report, (Def: Compar.lst):

 Execution control:
    List conversion coefficients for all subshells (Def. N):
    Calculate conversion coefficients for all transitions (Def. N):

 Processing started. Please wait.

      Processing a new data set
        1 : 172YB    172LU EC DECAY (6.70 D)
      104 : 172YB  G 155.87    7 0.032    7 M1(+E2)  0.7     LT   0.90   6
      107 : 172YBS G KC=0.72 8$LC=0.139 18$MC=0.032 5$NCC+=0.0085 12
<W> Non-standard data will be over-written
      109 : 172YB  G 174.671    190.180    8
      112 : 172YB  G 348.83     220.015    11
      113 : 172YB  G 596.75     150.102    23
      114 : 172YB  G 604.65     190.050    23
      115 : 172YB  G 990.75     150.12     6 D,E2
<W> Valid but NON-unique multipolarity. Calculation could not be performed.
      ...
      ...
     1265 : 172YB  G 1932.0     2 0.0019  5
     1267 : 172YB  G 2211.4     2 0.0034  6
 BrIcc finished processing BA1978Bo18.ens
 Processed:
    #DataSets     :        1
    #AllRecords   :     1269
    #GammaRecords :      286
    #Errors       :        0
    #Warnings     :       23
 Skipped:
    #DataSets     :        0
```

FIG. 7: BRICC – ENSDF tool terminal dialog.

Calculate conversion coefficients for all transitions (Def. N): The default is
to only calculate the conversion coefficients when a definite set of conversion
coefficients may be obtained; see the discussion on warnings below when BrIcc is
unable to do this and Table IV for examples of when this will be done. To obtain
a table of the E1-E5 and M1-M5 conversion coefficients for transitions with an
unknown multipolarity or non-unique multipolarity answer Yes (Y). Note that for
those transitions where a definite set of conversion coefficients may be obtained
the output will remain unchanged from the default and new records will still be
generated.

The program will process all data sets in the ENSDF file, except the IONIZED ATOM, COMMENTS and REFERENCES data sets. In the calculation report gamma–rays of a data set will be listed by increasing transition energy for each data set. (**NOTE:** BrIcc will create a binary file, BrIcc.tmp to store temporarily calculation reports.)

Different type of messages are given on the console window and in the calculations report file. These messages are designed to inform the evaluator and to assist to resolve conflicts or errors in the ENSDF file.

$< I >$ For information only. Calculations of new ICC's are carried out and new **G** and **s G** cards are generated.

$< W >$ Warnings are given if the ENSDF records are correct, but some of the fields contain non-unique information or, in some cases, when calculations of the ICC values could not be carried out this is indicated in the message. For example the **M** field contains $D+Q$, or transition energy (including its uncertainty) is outside the range of BrIcc tables.

$< E >$ An error is detected either on the **G**, or **G**–continuation, or on the **IDEN**tification card. As the program progressively scans through these records, the rest of the record will not be scanned.

$< F >$ Reserved for indicating, that BrIcc encountered an internal programming error. In such a case please forward the ENSDF data set and the error message to the authors.

C. BRICC – ENSDF utility to MERGE records

This program merges the new (corrected) **G**-records with the input ENSDF data set to create an updated data set.

```
bricc BA1978Bo18.ens merge<CR>
          BrIcc v2.0 (22-Sep-2005) calculates conversion coefficients
                (for electron conversion and pair production)
                        and E0 electronic factors
                    using cubic spline interpolation
          Theoretical Dirac-Fock conversion coefficients based on
              the so-called "Frozen Orbital" approximation


 Input & Data Files:
   Index file: C:\Program Files\BrIcc\BrIccFO.idx
   ICC file: C:\Program Files\BrIcc\BrIccFO.icc
   New G/SG cards, (Def: Cards.new):
   Output file of merged old and new cards, (Def: Cards.mrg):
 Merge operation completed!
```

FIG. 8: BRICC – ENSDF merge tool terminal dialog.

Program execution: `BRICC` *ENSDF-file* `merge<CR>`.

The ENSDF file name is passed as program argument.

WARNING: The input *ENSDF* file should not be modified before running the code in the MERGE mode.

Input file: File of new **G**-records created by BRICC. Before running the merge utility, one cane delete unwanted **G**-records. Default file: CARDS.NEW

Output files: Updated file in ENSDF format with new **G**-records inserted into the designated position. Default file: CARDS.MRG

NOTE: The ENSDF output files generated by HSICC and BRICC are not identical because (a) the conversion coefficient values are different; and (b) in the latter case a number of new quantities, for example **IPC**, are on the new **S G** cards.

Terminal dialog: (see Fig. 8)

VIII. TESTING OF THE BRICC PROGRAM PACKAGE

To provide a test of the ENSDF tool portion of BrIcc a subset of data was extracted from the ENSDF database at the NNDC in September 2004. This consisted of all IT decay data sets (total of 1773 transitions) and the $\beta-$ or electron-capture data set containing the most GAMMA records for each Z (total of 17637 γ's). It was felt that the IT data would provide a good test of the higher multipolarities and lower γ-ray energies and the $\beta-$ or electron-capture data should provide higher γ–ray energy testing. The data were processed using version 1.2 of BrIcc (September 12, 2004, using the *'No Hole'* approximation). The *Compar.lst* output from the program was parsed to obtain the original input and new output values of the total and K through NC+ shell conversion coefficients. All γ-rays where the total conversion coefficient (α_{tot}) was missing from the input or new output were excluded from further testing. The ratios of the ENSDF total conversion coefficient to the BrIcc total conversion coefficient were analyzed to identify possible problems in the BrIcc program. This consisted of looking at data for ratios that were outside the range of 0.9 through 1.1. Where available, the results from version 1.13f of HSICC (October 9, 2001) were used as an aid in the analysis. This process consisted of several parts:

1. If BrIcc and HSICC were in good agreement or there were no HSICC data, the original ENSDF data were looked at.

2. If an obvious error was found in ENSDF, the data were excluded from the comparison. If there was explicit documentation that the ENSDF conversion was anomalous, the data were retained (the largest ratio was an anomalous E1 with a value of 8.1). If no obvious errors were found in ENSDF and no problems could be identified in BrIcc, the data were also retained.
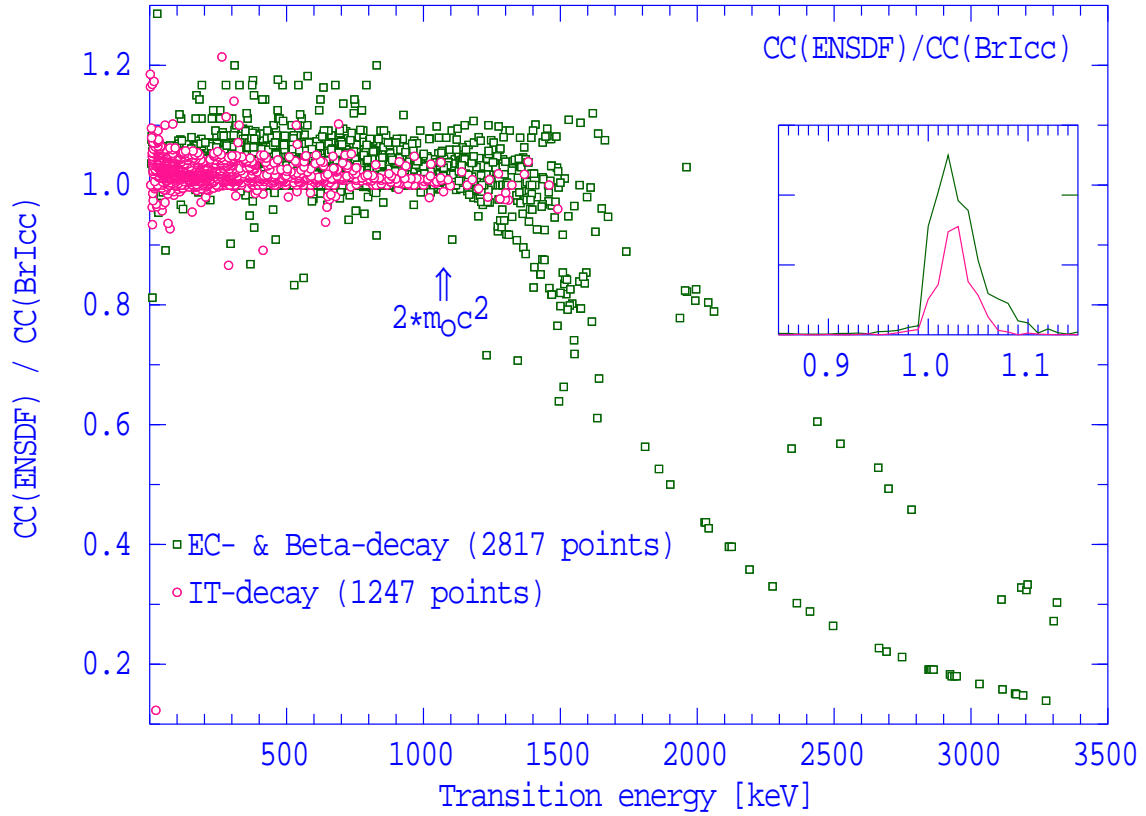
3. The BrIcc.lst output was checked if:

FIG. 9: Comparison of total conversion coefficients nuclear transitions of selected EC and β–decay (squares) and IT–decay (circles) data sets from the ENSDF data file compared with values calculated using BrIcc. The insert shows the frequency distribution of the CC(ENSDF)/CC(BrIcc) ratios.

(a) If BrIcc and HSICC values were discrepant.

(b) If HSICC data were not available and no obvious errors could be identified in the ENSDF data.

Identified problems were remedied in the program and were excluded from further comparison. Other cases were analyzed for some generic characteristics. Two of these are:

(a) Round-off problems. These typically occurred for M1,E2 and M1+E2 transitions with no mixing ratios resulting in an uncertainty greater than 25 in the last two significant digits and are grouped in the 1.1 to 1.2 range.

(b) Internal electron-positron pair formation. Above the pair production threshold ($E_\circ = 2m_ec^2$), the ratios started descending below 1.0 in a fairly consistent manner as a function of increasing E_γ. This appears to be caused by the internal pair coefficient becoming dominant as a function of increasing energy. Also, with a few exceptions, it was noticed that the E1 and M1 transitions were grouped

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into two distinct patterns with the M1 transition ratios higher than the E1 and both decreasing in a consistent manner.

The final set of data from the above analysis is shown in Fig. 9.

IX.   INSTALLATION AND DEVELOPMENT NOTES

The BLDBRICC and BRICC programs have been developed and extensively tested using Fortran 90/95 compilers on Win32 (CVF 6.6c), Linux (Lahey–Fujitsu LF95 and Intel F90) and UNIX (Digital F90) systems. Special considerations were given to avoid using system specific routines. In some places so–called compiler directive structures were used to adopt platform specific features.

External libraries used to develop the code included:

NSDFLIB library Nuclear Structure Data File Library, developed by the National Nuclear Data Center, Brookhaven National Laboratory and can be downloaded from http://www.nndc.bnl.gov/nndcscr/ensdf_pgm/nsdflib/

F2KCLI library a free implementation of the proposed Fortran F2003 command line interface, developed by Interactive Software Services Ltd. and can be downloaded from http://www.winteracter.com/f2kcli

On Windows platform the f2kcli.f90 source code has been modified, as the program failed to detect embedded blank character between double quotation (') marks. The modified version of the source code (f2kcli.f90) is now in the source directory.

X.   OBTAINING BRICC V2.0

The BrIcc program package can be obtained from the following web site: http://www.nndc.bnl.gov/nndcscr/ensdf_pgm/analysis/BrIcc/

The BRICC distribution packages contain the following files:

BrIcc.exe - binary executable file

BrIccFO.icc - binary ICC data file

BrIccFO.idx - binary pointer (lookup) file

BrIccManual.pdf - program manual (this document)

A.   Windows systems

The programs are compatible with Win9x/NT/ME/2000/XP operating systems. The self-extracting program archive will install the BrIcc program, the data files and the manual into a directory which can be selected during installation. It will create a BrIcc program group. On Windows NT, ME, 2000 and XP operating system the installation script will also set the 'BrIccHome' and 'Path' environment variables. On Windows 95 and 98 platforms the following two lines have to be added to the Autoexec.bat file:

```
set BrIccHome=<InstallDir>
set Path=%Path%;<InstallDir>
```

<InstallDir> is the directory where the program has been installed.

Due to different implementations of the command prompt, on Windows 95 and 98 systems the console buffer is limited to a maximum of 50 lines. To locate the data file the BrIcc program use the *BrIccHome* environment variable pointing to the directory, where the program and the data files are. In a typical installation, this directory is $C:\backslash Program\,Files\backslash BrIcc$. To enable the execution of BrIcc on the Command Prompt window from any working directory, the installation directory should be included into the Path variable.

To upgrade the program, please uninstall the previous version using the 'Uninstall' link provided in the BrIcc program group.

To test the program first test that the BrIccHome environment variable has been correctly set. On a Command Prompt (DOS window) to test the environment variables type

```
SET<CR>
```

and to test the path variable type

```
PATH<CR>.
```

To launch BrIcc from the *Start/Programs/BrIcc* menu or on a Command Prompt type

```
BrIcc<CR>
```

.

Do not forget to adjust the width of the screen to print long (117 character) lines.

B.   Compaq Tru64 UNIX and Linux

The installation procedure is almost identical for both Compaq Tru64 UNIX and Linux operating systems.

Create the main directory for the programs (for example `/usr/local/bin/bricc`). then download the distribution package, a tarred, gzipped file onto that directory. Un-tar and un-zipp all program and data files into this directory. BrIcc requires an environment variable BrIccHome to be set in order to locate the data files. Use the following shell commands to set the environment variables, on Digital Unix systems:

```
setenv BrIccHome /usr/local/bin/bricc
```

and on Linux systems:

```
export BrIccHome=/usr/local/bin/bricc.
```

To test the program on the console window type *BrIcc< CR >*. Adjust the width of the screen to print long (117 character) lines.

XI. ACKNOWLEDGEMENT

TABLE II: ENSDF **G** record containing information on the
nuclear transitions. Taken from J.K. Tuli [2001TuAA]

Field	Name	Description
1-5	NUCID	Nuclide identification
6		Blank or continuation character
7		Must be blank
8	G	Letter G is required
9		Must be blank
10-19	E	Energy of the γ-ray in keV
20-21	DE	Standard uncertainty in E
22-29	RI	Relative photon intensity
30-31	DRI	Standard uncertainty in RI
32-41	M	Multipolarity of transition
42-49	MR	Mixing ratio, δ.
50-55	DMR	Standard uncertainty in MR
56-62	CC	Total conversion coefficient
63-64	DCC	Standard uncertainty in CC
65-74	TI	Relative total transition intensity
75-76	DTI	Standard uncertainty in TI
77	C	Comment FLAG
78	COIN	Letter C denotes placement confirmed by coincidence. Symbol ? denotes questionable coincidence.
79		Blank
80	Q	The character ? denotes an uncertain placement

TABLE III: ENSDF GAMMA continuation record. Taken from J.K. Tuli [2001TuAA]

Field	Name	Description
1-5	NUCID	Nuclide identification
6		Any alphanumeric character other than 1.
		NOTE: 'S' is reserved for records not shown
		in the Nuclear Data Sheets
7		Must be blank
8	G	Letter G is required
9		Must be blank
10-80	DATA	Allowed quantities

The general form of a data entry as described on p. 33 of [2001TuAA] is:

$$< quant >< op >< value > [< op >< value >][< ref >]\$$$

G continuation record – any character other than 1 or S in column 6

E, DE^a, RI, DRI, M, MR^a, DMR^a, CC^a, DCC^a, TI, DTI, C, COIN, Q, BE1, BE2, ...; BE1W, BE2W, ...; BM1,BM2, ...; CE, CEK, CEL, ...; CEL1, ...; ECC^a, EKC^a, ELC^a, $EL1C^a$, $EL2C^a$, $EKLC^a$, $EKL1C^a$...; FL, FLAG

S G records – character 'S' in column 6

BrIcc will scan the existing **'S G'** records and validate and will replace the Data entries, if they comply with the following rules:

(a) **TI** not given in **G** record and **M** is known

On the first **S G** record:

CC, **KC**, **LC**, **MC**, **NC+** (electron conversion coefficients)

On additional **S G** records:

NC, $\mathbf{OC}^b$, $\mathbf{PC}^b$, $\mathbf{QC}^b$ and $\mathbf{RC}^b$ (electron conversion coefficients) and **IPC** (pair conversion coefficient^b)

Obsolete data entries also verified and will be removed, including:

MC+, **M+** and **N+**.

(b) **TI** given in **G** record and **M** is known

On the first **S G** record:

CC and

K/T, **L/T**, **M/T**, **N+/T** (intensity ratios)

On additional **S G** records:

N/T, **O/T**, **P/T**, **Q/T** and **R/T** and

IP/T (internal pair to total intensity ratio^b)

Obsolete data entries also verified and will be removed, including:

M+/T and a warning will be issued.

Any other data entry or text will be copied onto new **S G** records and will be inserted as new.

---

^{a} – *BrIcc will read and interpret its numerical value.*

^{b} – *To be declared in ENSDF dictionary and manual.*

TABLE IV: Typical values of the multipolarity (M), Mixing ratio (MR) and uncertainty (DMR) fields of the **G** record

M	MR	DMR	Multipolarity assignment
M1			Definite M1
(M1)			Uncertain M1
[E2]			Assumed E2
M1+E2	2.5	7	M1 plus E2, definite
			$\delta(E2/M1) = 2.5\,(7)$, symmetric uncertainty
M1+E2	+0.014	+15-12	Mixed M1 plus E2, definite,
			$\delta(E2/M1) = +0.14^{+15}_{-12}$, asymmetric uncertainty
M1+E2	2.5	LE	M1 plus E2, definite
			$\delta(E2/M1) \leq 2.5$, upper limit
[M1,E2]			Assumed mixed M1 plus E2,
			assumed $\delta(E2/M1) = 1$ with no uncertainty
E1+M2+E3	+0.012	+6-4	Mixed E1 plus M2 plus E3, definite,
			$\delta(M2/E1) = +0.012^{+6}_{-4}$
			(E3 multipolarity component omitted)
[E1,M2,E3]			Assumed mixed E1 plus M2 plus E3,
			assumed $\delta(M2/E1) = 1$
			(E3 multipolarity component omitted)
E0+M1+E2	+2.7	+3-1	Mixed E0 plus M1 plus E2, definite,
			$\delta(E2/M1) = +2.7^{+3}_{-1}$
			$q(E0/E2) = 0.24\,(3)$ given in the GAMMA cont. record[a]

[a] *To be declared in ENSDF dictionary and manual.*

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